

A puzzle in quantum dynamics

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Abstract: The textbook treatment in that the wave function of a dynamical system is expanded in an eigenfunction series is investigated. With help of an elementary example and some mathematical theorems, it is revealed that in terms of solving the time-dependent Schrödinger equation the treatment involves in divergence trouble. The root reason behind the trouble is finally analyzed.

PACS numbers: 03.65-w

Solutions of the time-dependent Schrödinger equation, formal ones and numerical ones, are of considerable interest in the past and in the present. It is recognized that they are related to many interesting and essential dynamical processes in the quantum realm.

Being aware of difficulties with solving the time-dependent Schrödinger equation directly, the textbook treatment takes the detour-type approach in that a wave function is expanded in an eigenfunction series and thus the dynamics of coefficients of the series, instead of that of the wave function, becomes the focus of the theory[1]. The procedure was put forward initially by Dirac at the early time of quantum mechanics and has since been accepted as one of standard methods in many perturbative and nonperturbative approaches.

Though not enough attention was received, discussions and suggestions concerning the Dirac approach existed for decades[2][3]. In some of our recent papers, it was argued that even for today's physicists there were still things worth careful consideration[4]. The purpose of this paper is to examine the pure mathematical aspect of the subject. By the term "the pure mathematical aspect" we mean that (i) the foundation of solving the time-dependent Schrödinger equation, not any concrete perturbative procedure, will be of interest; (ii) only simple examples that can be investigated both numerically and analytically will be discussed; (iii) except the energy concept no physical arguments, particularly those of gauge, will be related.

The basic assumption of the standard treatment is that a system's wavefunction can be expanded in a series of the following form

$$\Psi(t, \mathbf{r}) = \sum C_n(t) e^{-iE_n t/\hbar} \Psi_n(\mathbf{r}), \quad (1)$$

where $C_n(t)$ stands for a coefficient that is a constant before the initial time and then becomes time-dependent after it and $\Psi_n(\mathbf{r})$ is one of the eigenfunctions satisfying the eigenvalue equation

$$H_0 \Psi_n(\mathbf{r}) = E_n \Psi_n(\mathbf{r}), \quad (2)$$

in which H_0 , according to the convention, represents the Hamiltonian of the system at the initial time. Provided that all eigenfunctions are adequately normalized, the coefficients of the expansion must obey the normalization condition

$$\sum_n^\infty |C_n(t)|^2 = 1. \quad (3)$$

Inserting (1) into the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H(t, \mathbf{r}) \Psi, \quad (4)$$

multiplying both the sides by $e^{iE_n t/\hbar} \Psi_n^*(\mathbf{r})$ and integrating the resultant equation term by term, we arrive at a set of coupled ordinary-differential equations

$$i\hbar \frac{dC_n}{dt} = \sum_l C_l V_{nl} \exp(i\omega_{nl}t), \quad (5)$$

where $\omega_{nl} = (E_n - E_l)/\hbar$ and V_{nl} stands for the matrix element of the Hamiltonian variation $V(t) \equiv H(t) - H_0$. It is almost unanimously believed that the equation set (5) is completely and exactly equivalent to the Schrödinger equation (4) and, at the same time, enjoys some advantages. One of the advantages is that the equation set appears to be numerically solvable and some efforts are indeed in this direction[3]. According to the customary thought, there is nothing to be discussed concerning the validity of (5) because (i) no approximation has been introduced; (ii) no perturbative procedure has been invoked; (iii) no physical interpretation has been imposed.

Nevertheless, we will, in this paper, show that the formalism outlined above is not truly reliable since the basic expansion (1) is not a mathematically well-behaved series.

Before discussing the issue in an abstract way, let's apply the standard formalism to a one-dimensional oscillator and see where it leads us to. The oscillator is assumed to have the Hamiltonian

$$H(t) = \frac{p^2}{2m} + \frac{S(t)}{2} k^2 x^2, \quad (6)$$

where

$$S(t) = \begin{cases} 1 & (t \leq 0) \\ 1 + \eta t & (0 < t < T) \\ 1 + \eta T & (t \geq T). \end{cases} \quad (7)$$

(Several other types of time-dependent Hamiltonians were also tried. The situations were all alike as far as the subject of this paper was concerned.) It is well-known that the system expressed by (6) is a simple harmonic oscillator before $t = 0$. The quantum state before $t = 0$ is expressed by

$$\sum_{n=0} C_{n0} e^{-i(n+1/2)\omega t} N_n(\alpha) H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}, \quad (8)$$

where $\omega = \sqrt{k/m}$, $\alpha = (mk/\hbar^2)^{1/4}$, $N_n = [\alpha/(\sqrt{\pi}2^n n!)]^{1/2}$ and H_n is the n th Hermite polynomial, which is governed by the iteration relation

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi) \quad (9)$$

with

$$H_0(\xi) = 1, \quad H_1(\xi) = 2\xi, \quad H_2(\xi) = 4\xi^2 - 2 \quad (10)$$

We will assume that the system is in the ground state before $t = 0$, namely we have

$$C_0(0) = 1 \quad \text{and} \quad C_n(0) = 0 \quad (n \neq 0), \quad (11)$$

and try to calculate the quantum state at the later times.

To make the numerical work as simple as possible, we set

$$\eta = 1, \quad T = 1, \quad m = 1, \quad k = 1, \quad \hbar = 1. \quad (12)$$

Under these conditions, the Hamiltonian variation $V(t)$ becomes

$$V(t) = \begin{cases} x^2 t/2 & (0 < t < T) \\ x^2/2 & (t \geq T). \end{cases} \quad (13)$$

By virtue of the iteration relation (9), we obtain the following relations

$$\langle 2j|x^2/2|2j\rangle = (j + 0.25) \quad (14)$$

and

$$\langle 2j|x^2/2|2j+2\rangle = 0.5 \times [(j+0.5)(j+1)]^{\frac{1}{2}}. \quad (15)$$

With the notation $C_n = C_n^r + iC_n^i$, the equation set (5) becomes

$$\begin{aligned} \frac{dC_{2j}^r}{dt} &= [C_{2j-2}^i \cos(2t) + C_{2j-2}^r \sin(2t)]V_{2j-2,2j} \\ &+ C_{2j}^i V_{2j,2j} + [C_{2j+2}^i \cos(2t) - C_{2j+2}^r \sin(2t)]V_{2j,2j+2} \end{aligned} \quad (16)$$

and

$$\begin{aligned} \frac{dC_{2j}^i}{dt} &= -\{[C_{2j-2}^r \cos(2t) - C_{2j-2}^i \sin(2t)]V_{2j-2,2j} \\ &+ C_{2j}^r V_{2j,2j} + [C_{2j+2}^r \cos(2t) + C_{2j+2}^i \sin(2t)]V_{2j,2j+2}\}, \end{aligned} \quad (17)$$

where j runs over all non-negative integers. Note that in the equations above any quantity having a negative subindex actually vanishes. Namely, $C_{-2}^r = C_{-2}^i = 0$ and $V_{-2,0} = 0$.

In numerical mathematics the Runge-Kutta algorithm[5] says that for a vector-type differential equation

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}, t), \quad (18)$$

we can construct the solution according to the formula

$$\mathbf{y}_{j+1} = \mathbf{y}_j + \frac{1}{6}(\mathbf{z}_1 + 2\mathbf{z}_2 + 2\mathbf{z}_3 + \mathbf{z}_4), \quad (19)$$

where

$$\mathbf{y}_0 = \mathbf{y}(t_0), \mathbf{y}_1 = \mathbf{y}(t_1), \dots, \mathbf{y}_j = \mathbf{y}(t_j), \dots, \quad (20)$$

with $t_j - t_{j-1} = h$, and

$$\begin{aligned} \mathbf{z}_1 &= h\mathbf{f}(\mathbf{y}_j, t_j) \\ \mathbf{z}_2 &= h\mathbf{f}(\mathbf{y}_j + \mathbf{z}_1/2, t_j + h/2) \\ \mathbf{z}_3 &= h\mathbf{f}(\mathbf{y}_j + \mathbf{z}_2/2, t_j + h/2) \\ \mathbf{z}_4 &= h\mathbf{f}(\mathbf{y}_j + \mathbf{z}_3, t_j + h). \end{aligned}$$

Although the algorithm proves very effective in classical mechanics[6], it encounters difficulties one by one in dealing with (16) and (17). Firstly, it is found that the number of involved variables, namely nonzero C_{2j}^r and C_{2j}^i , increases rapidly. At $t = 0$, only $C_0^r = 1$ is there. At $t = nh$, we have $(8n + 2)$ nonzero variables. Secondly, when the code, adapted to the increasing number of variables, is run in a computer, it is found that if the Hamiltonian $V(t)$ is relatively large, the normalization condition $\sum |C_n(t)|^2 = 1$ will soon be broken down. Figure 1 illustrates that the breakdown takes place within an oscillation cycle in respect to the perturbation described by (13) and $h = 0.001$. Thirdly, it is noted that whenever the normalization condition runs into difficulty, the average energy of the system

$$\langle E \rangle = \sum E_n |C_n(t)|^2 \quad (21)$$

tends to infinity in a similar way as shown in Figure 2. (The code is available if more details are interested.)

If we study the numerical calculation in an analytical manner, more puzzling things surface impressively. Equations (16) and (17) suggest that if the system is in the ground state initially, it will, at the next step, be

partly in the second excited state owing to the coupling of the coefficients. At the next next step, it will be partly in the fourth excited state. Since the Hamiltonian variation $V(t)$ (13) has a finite value as $t \rightarrow \infty$, the process will never terminate and the state of the system will vary forever. However, elementary quantum mechanics[7] asserts that the system will be settled in a stationary state after $t = T$. The contrast becomes more striking if we look at Figure 2, in which the “energy” curve rises and falls at the times $t > T = 1$ disregarding any theory about stationary states.

Another perplexing thing is related to energy more directly. According to the formulas (3) and (21), a ground-state system cannot lower its energy under any circumstances. The physical intuition, however, tells us a different story. For instance, if the Hamiltonian variation of our oscillator takes the following form

$$V(t) = -x^2 t/2 \quad (t > 0), \quad (22)$$

the system, in contrast to the system affected by (13), should lose its energy since, roughly speaking, the perturbation (22) makes the potential energy of the system smaller while leaving the kinetic energy unchanged.

We now try to work out the puzzle related to the title of this paper: Why does the standard formalism, derived from the Schrödinger equation in a seemingly rigorous way, suffer from so many difficult things? For our purposes, the analysis will be done almost entirely from mathematical consideration.

It should be pointed out that

$$e^{-iE_0 t/\hbar} \Psi_0(\mathbf{r}), e^{-iE_1 t/\hbar} \Psi_1(\mathbf{r}), \dots, e^{-iE_n t/\hbar} \Psi_n(\mathbf{r}), \dots \quad (23)$$

do not constitute an orthogonal-and-complete basis for a function $f(t, \mathbf{r})$. Consider our one-dimensional case again. Many functions, such as

$$t, (t + x), \cos(tx) e^{-\frac{1}{2}\alpha^2 x^2}, e^{tx} e^{-\frac{1}{2}\alpha^2 x^2}, \dots, \quad (24)$$

cannot be expanded in a series of the form (8). That is to say, the practice of expanding the solution of a Schrödinger equation in a series of eigenfunctions is originated from an intuitive physical idea rather than from a stringent mathematical analysis.

The major argument, which we wish to propose in this paper, is the following. Even if the wave function at any fixed time can be expanded in an eigenfunction series of the form

$$\sum C_n(t) \Psi_n(\mathbf{r}), \quad (25)$$

substitution of this expansion, or the equivalent series (1), into the time-dependent Schrödinger equation is still a questionable procedure. As a matter of fact, there indeed exist mathematical theorems restricting the use of infinite series[8]. One of them states that only a series converging uniformly can safely be integrated term by term. Another of them indicates that to differentiate a series term by term the resultant series has to be uniformly convergent. An inspection can tell us that any known eigenfunction series, if given as a truly infinite one, behaves poorly in this respect and cannot be safely used in the time-dependent Schrödinger equation. To see this in an example, apply the standard treatment to the series (8). Assume that in the series

$$C_{n0} = \frac{\sqrt{6}}{\pi(n+1)}, \quad \text{such that} \quad \sum |C_{n0}|^2 = \frac{6}{\pi^2} \sum \frac{1}{(n+1)^2} = 1. \quad (26)$$

By taking the time derivative, the left side of the Schrödinger equation becomes

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{\sqrt{6}\hbar\omega}{\pi} e^{-\frac{1}{2}\alpha^2 x^2} \left[\sum_n \frac{n+1/2}{n+1} e^{-i(n+1/2)\omega t} N_n(\alpha) H_n(\alpha x) \right]. \quad (27)$$

For this step and the next step to make sense, in which the expression has been differentiated and will be integrated term by term, it is necessary to ensure the uniform convergence of the series included in the square bracket above. (Note that the common factor $e^{-(\alpha x)^2/2}$ is not relevant to the treatment term by term.) By setting $t = 0$, this series becomes

$$\sum_n \frac{n+1/2}{n+1} N_n(\alpha) H_n(\alpha x) \sim \sum_n \frac{(2\alpha x)^n}{(2^n n!)^{1/2}}, \quad (28)$$

whose value rises very fast for large x (faster than $e^{2\alpha x}$). A simple analysis tells us that the series cannot be uniformly convergent since it has no upper limit on its domain.

At this stage, it is desired to have explanation for the fact that the series form

$$\sum C_{n0} e^{-iE_n t/\hbar} \Psi_n(\mathbf{r}), \quad (29)$$

where C_{n0} are pure time-independent constants, has safely been used for almost all stationary states. We believe that there are two facts responsible for it. The first one is that for practical cases the initial expansion of (29) takes the form

$$\sum_{n=0}^N C_{n0} \Psi_n(\mathbf{r}), \quad (30)$$

where N is a finite number. The finiteness of the series is due to the fact that high-energy eigenfunctions are related to the wave function in the very remote regions, which are usually of no interest for the problem, in which a fixed accuracy is set up at the very beginning. The second one is that each term in (30) evolves in the Schrödinger equation independently (no coupling), and therefore the series, if finite initially, keeps finite in all treatments. Keeping these facts in mind, one may say that a stationary wave function can indeed be expanded in a series of eigenfunctions (with limitations still, see Ref. 4).

The discussion above has almost already manifested that things will be different for nonstationary cases. We may still express the dynamical wave function as a finite series at the initial time, but the series soon becomes a truly infinite one. The strong coupling, as (5) exhibits, tends to make each of the coefficients have a significant value. This is disastrous in view of that any truly infinite eigenfunction series suffers seriously in the time-dependent Schrödinger equation, as has been unveiled.

From a slightly different viewpoint, we can also see that the expansion (1) cannot work smoothly. It is obvious that after the initial time the eigenfunctions defined by H_0 are no longer adequate eigenfunctions and the eigenfrequencies defined by $\omega_n = E_n/\hbar$ are no longer adequate eigenfrequencies. If we forcefully express the dynamical wave function in a series constructed from these “out-of-date” eigenfunctions and “out-of-date” eigenfrequencies, the coefficients of the series have to adjust themselves violently. Since the large scale (the entire space) and the fast variation (represented by $e^{-in\omega t}$) get involved, the adjustment has to be so violent that the normalization condition $\sum |C_n|^2 = 1$ will definitely break down.

We proposed two alternatives to the standard treatment[9][10]. One is based on a perturbative approach and the other is based on a nonperturbative approach. In the nonperturbative approach, with help of “intermediate” eigenfunctions and eigenfrequencies a general procedure of solving the time-dependent Schrödinger equation is constructed.

Mathematical discussion with Professor Qihou Liu is gratefully acknowledged. The work is partly supported by the fund provided by Education Ministry, P.R. China.

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Figure captions

Fig. 1, The time behavior of the coefficients in terms of the normalization condition. Note that the period of the oscillator is 6.28 since $\omega = 1$.

Fig. 2, The time behavior of the coefficients in terms of the average energy.

Figure 1

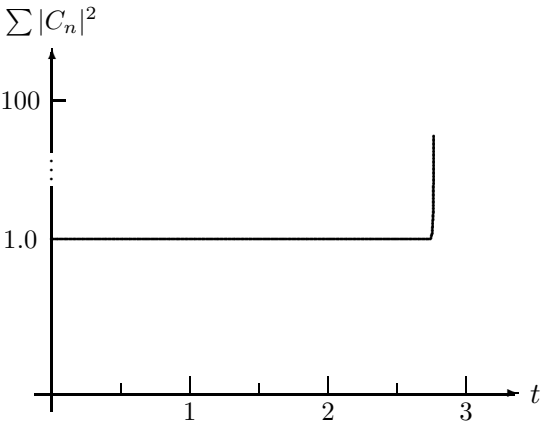


Figure 2

